Correlation effects on resonant tunneling in one-dimensional quantum wires

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We study resonant tunneling in a Luttinger liquid with a double barrier enclosing a dot region. Within a microscopic model calculation the conductance G as a function of temperature T is determined over several decades. We identify parameter regimes in which the peak value $G_p(T)$ shows distinctive power-law behavior. For intermediate dot parameters G_p behaves in a non-universal way.

A decade ago resonant tunneling through a double barrier embedded in a Luttinger liquid was intensively studied theoretically.[1, 2, 3] At temperature $T = 0$, in the limit of an infinite system, and for symmetric barriers the conductance G was predicted to show a series of infinitely sharp resonances if the gate voltage V_g applied to the dot region is varied.[1] For spinless fermions, on which we focus, the peak conductance G_p at resonance voltage V_g^r is given by e^2/h if the interacting wire (denoted "the wire" in the following) is connected by "perfect" contacts to non-interacting semi-infinite leads as will be the case here. Increasing T resonances are still present but acquire a non-vanishing width $w(T) \propto T^{1-K}$,[1] with the interaction dependent Luttinger liquid parameter K ($K = 1$ for non-interacting particles). We here restrict ourselves to the case $1/2 \leq K \leq 1$. For $\Delta V_g = |V_g - V_g^r| \neq 0$, $G(T)$ scales to zero as $T^{2\alpha_B}$,[1] with $\alpha_B = 1/K - 1$. This also holds for an asymmetric double barrier regardless if the conductance is evaluated at or off resonance.

Using second order perturbation theory in the barrier height the $T > 0$ deviations of $G_p(T)$ from e^2/h were determined to scale as T^{2K}.[2] At further increasing T a regime of uncorrelated sequential tunneling (UST) was predicted[4] based on a perturbative analysis in the inverse barrier height, where $G_p(T) \propto T^{\alpha_B - 1}$ and $w(T) \propto T$. This regime is bounded from above by the level spacing of the dot $\Delta_D = \pi v_F/N_D$, where v_F denotes the Fermi velocity, N_D the number of lattice sites in the dot, and the lattice constant was chosen to be 1. Within the same perturbative approach and for $\Delta_D < T < B$, where B is the bandwidth, $G_p(T)$ increases as $T^{2\alpha_B}$ for increasing T.[2, 4] In contradiction to the temperature dependence following from UST, in transport experiments on carbon nanotubes a suppression of G_p with decreasing T was observed for $T \lessapprox \Delta_D$.[5] Using another approximation scheme "correlated sequential tunneling" (CST) was predicted to replace UST.[6] It leads to $G_p \propto T^{2\alpha_B - 1}$ which was argued to be consistent with the experimental data. This consideration has stimulated a number of theoretical works.[7, 8, 9, 10]

Quantum Monte Carlo (QMC) results[10] for $G_p(T)$ were interpreted to be consistent with CST for $T \lessapprox \Delta_D$.

In Refs. [8, 9] a "leading-log" type of resummation for the effective transmission at the chemical potential was applied and led to important insights. In this approach no signature of CST was found, but it was criticized for only being valid in the limit of small interaction. That the "leading-log" method indeed does not capture all interesting interaction effects away from $K \to 1$ can be seen considering the single barrier case for which the conductance for different temperatures and barrier heights can be collapsed onto a single curve by using a one-parameter scaling ansatz.[1] While the resulting scaling function is known to depend on K,[1] the "leading-log" approach leads to the non-interacting $K = 1$ scaling function independently of the interaction strength chosen.[11, 12]

In Ref. [7] a $N_D = 1$ double barrier model in which chiral fermions carry the current was treated for $K = 1/2$ by refermionization. After fine tuning the Coulomb coupling across the barriers $G_p(T)$ was predicted to show the non-interacting behavior, i.e. $e^2/h - G_p(T) \propto T^2$ for $T \to 0$ and $G_p(T) \propto T^{-1}$ in the UST regime. This finding is surprising and not supported by any of the results obtained for more general models using the above mentioned methods. The physics of this particular model thus seems to be non-generic.

We study the problem applying the fermionic functional renormalization group (fRG) method to the model of spinless fermions on a lattice with hopping $t = 1$ and nearest neighbor interaction $U > 0$ at half filling.[12, 13, 14] By using a method which can be applied for any barrier height and shape but is restricted to weak to intermediate interactions our study is complementary to the one using perturbation theory in either the barrier heights or the inverse barrier heights.[2, 4] Considering the single barrier case and comparing with exact asymptotic and numerical results we have shown previously that our method leads to meaningful results even for fairly large $U \lessapprox 2$.[12, 13, 14] In Ref. [12] it was shown that for $K = 1/2$ our data for G collapse onto the exactly known scaling function of the local sine-Gordon model.[1] Without any further approximations the fRG can be applied to the double barrier problem and we thus expect that regimes with universal power-law scaling and the related exponents can reliably be determined. Accurate results can also be obtained for regions of dot parameters not investigated so far in which $G_p(T)$ shows non-universal behavior, i.e. a behavior which cannot be characterized as a power-law scaling with an exponent expressible in terms of K. Studying these turns out to be relevant for the

interpretation of the QMC data[10] and the experimental results.[5] In contrast to the other methods which can only be applied in certain temperature ranges the fRG provides reliable results for $G(T)$ on all energy scales. For large barriers and large as well as small dots we identify a variety of temperature regions in which $G_p(T)$ shows distinctive power-law behavior with different exponents expressible in terms of K. For intermediate barrier height, intermediate dot sizes, and $T \lessapprox \Delta_D$, $G_p(T)$ decreases with decreasing T. The behavior of $G_p(T)$ in this temperature regime depends on N_D and the height of the barriers and is thus non-universal. Whereas our results are consistent with the QMC data, we do not observe signatures of CST.

The model is given by the Hamiltonian

$$H = -\sum_{j=-\infty}^{\infty} \left(c_j^\dagger c_{j+1} + \text{h.c.} \right) + V_l n_{j_l-1} + V_r n_{j_r+1} + V_g \sum_{j=j_l}^{j_r} n_j + \sum_{j=1}^{N-1} U_j \left(n_j - \frac{1}{2} \right) \left(n_{j+1} - \frac{1}{2} \right) , \quad (1)$$

with $1 \ll j_l < j_r \ll N$, in standard second-quantized notation. The lattice can be divided in three parts: (1) the wire with nearest neighbor interaction U_j across the bonds $(j, j+1)$ with $j \in [1, N-1]$; (2) the dot (embedded in the wire) on sites $j \in [j_l, j_r]$ ($N_D = j_r - j_l + 1$) which can be shifted in energy by the onsite energy V_g and is separated by barriers of strength $V_{l/r}$ from the rest of the lattice; (3) the non-interacting leads on sites $j < 1$ and $j > N$. Besides site impurities we also consider hopping impurities as barriers. In this case the interaction [in the last term of Eq. (1)] and hopping [in the first term of Eq. (1)] across the bonds $j_l - 1, j_l$ and $j_r, j_r + 1$ are set to zero. Furthermore the second and third terms in the first line of Eq. (1) are replaced by $-t_l c_{j_l-1}^\dagger c_{j_l} - t_r c_{j_r}^\dagger c_{j_r+1} + \text{h.c.}$ with the reduced hopping matrix elements $t_{l/r} < 1$. As in the other theoretical studies mentioned we avoid effects of the contacts. We thus model "perfect" contacts by a smooth spatial variation of the interaction U_j close to the sites 1 and N. Starting at site 1 in our calculations the interaction was turned on in an arctan-shape over the first 100 sites and similarly turned off approaching site N.[12] For $T = 0$, vanishing barriers, and up to $N = 10^4$ this gives $1 - G/(e^2/h) < 10^{-6}$. The constant bulk value of the interaction is denoted by U.

In linear response and the absence of vertex corrections the conductance is given by[15]

$$G(T) = -(e^2/h) \int_{-2}^{2} |t(\varepsilon, T)|^2 \, \partial_\varepsilon f(\varepsilon/T) \, d\varepsilon \, , \quad (2)$$

with $|t(\varepsilon, T)|^2 = (4 - \varepsilon^2) |\tilde{G}_{1,N}(\varepsilon, T)|^2$ and f being the Fermi function. The one-particle Green function $\tilde{G}_{i,j}$ has to be computed in the presence of interaction and leads. To this end we extend a recently developed fRG scheme, which has been shown to provide excellent results at $T = 0$,[12, 13, 14] to finite temperatures. The starting point of this approach is an exact hierarchy of differential flow equations for the self-energy Σ^Λ and higher order vertex functions, with an energy cutoff Λ as the flow parameter. The hierarchy is truncated by neglecting n-particle vertices with $n > 2$, and the 2-particle vertex is parametrized approximately by a renormalized nearest neighbor interaction U^Λ. The spatial dependence of the renormalized impurity potential, described by Σ^Λ, is however fully kept. This procedure is perturbative in the 2-particle interaction, but non-perturbative in the impurity strength. Within our approximate scheme Σ^Λ has no imaginary part, which implies the vanishing of the vertex corrections to the conductance formula (2).[15] The Green function $\tilde{G}_{1,N}$ entering Eq. (2) is obtained from the Dyson equation with $\Sigma^{\Lambda=0}$.

As a test of our method at finite T we first discuss results for the single barrier problem. We find the expected scaling behavior of the conductance (for an example see the solid line in the upper panel of Fig. 2).[1, 12] From the suppression of $G(T) \propto T^{2\alpha_B}$, the exponent α_B can be read off. Within our truncation scheme we obtain an approximation $\alpha_B^{\text{RG}}(U)$ for $\alpha_B(U)$. Consistent with the exponents of the $1/N$-scaling determined in Ref. [12] at $T = 0$ we find $\alpha_B^{\text{RG}}(0.5) = 0.165$, $\alpha_B^{\text{RG}}(1) = 0.35$, and $\alpha_B^{\text{RG}}(1.5) = 0.57$ in good agreement with the exact exponents $\alpha_B(0.5) = 0.1608$, $\alpha_B(1) = 1/3$, and $\alpha_B(1.5) = 0.5398$ known from the Bethe ansatz solution of the bulk model.[16]

For the double barrier problem we start the discussion with the case of strong, symmetric barriers. In Fig. 1 $G(V_g)$ is shown for $N_D = 6$, $U = 0.5$, $V_{l/r} = 10$ and different T. In all figures the wire length is chosen to be $N = 10^4$ sites in rough agreement with the length of carbon nanotubes accessible to transport experiments.[5] For sufficiently small T resonance peaks are clearly developed. For $T \to 0$, $G_p(V_g^r)$ tends towards e^2/h. Because of $N < \infty$ even at $T = 0$ the peaks have finite width. For all peaks the $T = 0$ width scales to zero as $N^{K^{\text{RG}}-1}$,[1] with the fRG approximation K^{RG} for K. The different height and width of the peaks at fixed T is a finite band effect. In the following we always study the behavior of the resonance closest to $V_g = 0$. We have verified that $G_p(T)$ for the other peaks shows a similar T-dependence.

In the upper panel of Fig. 2 $G_p(T)$ is shown for $U = 0.5$, $V_{l/r} = 10$, and $N_D = 2, 6, 100$. The lower panel contains the logarithmic derivative of $G_p(T)$ from which the exponents of possible power-law behavior can be read off directly. Several temperature regimes can be distinguished. For T larger than the bandwidth, $G_p(T) \propto T^{-1}$. For $T < \Delta_D$, marked by arrows in Fig. 2, down to a lower bound T^* discussed below we find $G_p(T) \propto T^{\alpha_B^{\text{RG}}-1}$ as indicated in the lower panel of Fig. 2 by the dashed line. This is the regime of UST,[4] in which the integral Eq. (2) leading to $G_p(T)$ is dominated by a single peak of

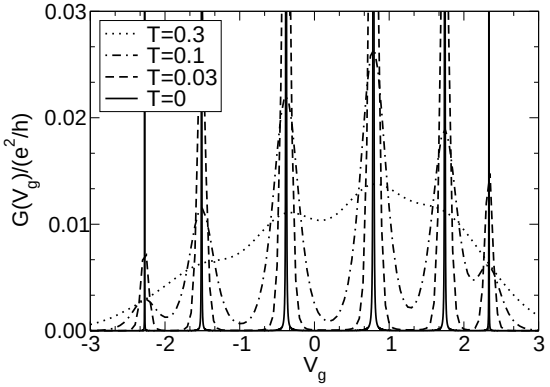

FIG. 1: The conductance as a function of gate voltage for $N_D = 6$, $U = 0.5$, $V_{l/r} = 10$, $N = 10^4$, and different T.

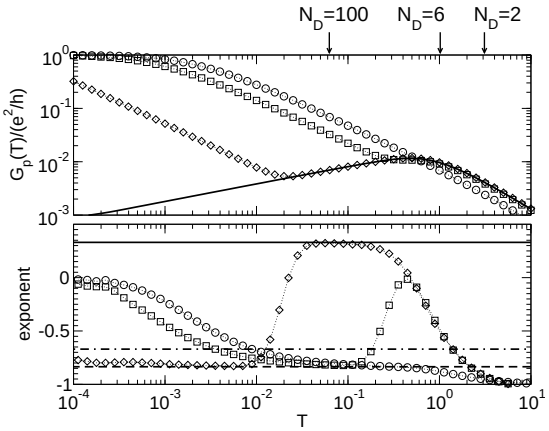

FIG. 2: Upper panel: $G_p(T)$ for $U = 0.5$, $N = 10^4$, $V_{l/r} = 10$, and $N_D = 2$ (circles), 6 (squares), and 100 (diamonds). The arrows indicate Δ_D. The solid curve shows $G(T)/2$ for a single barrier with $V = 10$ and $U = 0.5$, $N = 10^4$. Lower panel: Logarithmic derivative of $G_p(T)$. Solid line: $2\alpha_B^{\rm RG}$; dashed line: $\alpha_B^{\rm RG} - 1$; dashed-dotted line: $2\alpha_B^{\rm RG} - 1$.

$|t(\varepsilon, T)|^2$, but T is still much larger than the width of this peak. Peaks in $G_p(V_g)$ are clearly separated and the width $w(T) \propto T$ can be read off. The size of the UST regime grows with increasing N_D and shifts towards smaller T. For $N_D \geq 4$ we find non-monotonic behavior of $G_p(T)$. For $N_D \gtrapprox 30$ the region of decreasing conductance (with decreasing T) can be described by a power-law with exponent $2\alpha_B^{\rm RG}$ (solid line in the lower panel of Fig. 2).[2] For these T many peaks of $|t(\varepsilon, T)|^2$ contribute to the integral. For $V_{l/r} \gg 1$ and $N_D \gg 1$, i.e. in the parameter regime with distinctive power-law scaling, the non-monotonic behavior can be understood using Kirchhoff's law. The solid line in the upper panel of Fig. 2 displays $G(T)/2$ obtained for a single barrier with $V = 10$ and $U = 0.5$. The comparison shows that the conductance of the double barrier problem for T up to the local minimum can be determined by adding up resistances of the related single barrier case. We do not observe indications of CST with exponent $2\alpha_B^{\rm RG} - 1$, shown as the dashed-dotted line in the lower panel of Fig. 2. For $T \to 0$, $G_p(T)/(e^2/h)$ saturates at 1. Due the finiteness of the wire for $T \ll \Delta_W$, with $\Delta_W = \pi v_F/N$, we find $1 - G_p(T)/(e^2/h) \propto T^2$. For small N_D and intermediate to small barriers at increasing T this behavior is followed by a regime with $1 - G_p(T)/(e^2/h) \propto T^{2K^{\rm RG}}$.[2] All the above scaling regimes we also find for $U = 1$ and 1.5.

Temperature regimes with power-law behavior and the same scaling exponents were obtained using a field theoretical model and perturbation theory in $V_{l/r}$ as well as $1/V_{l/r}$.[2, 4] The agreement of the results obtained from two complementary approximate methods and for different models constitutes a strong argument for the correctness of the physics obtained. These considerations put very tight limits on the parameters for which a scaling regime with exponent $2\alpha_B - 1$ could occur.[6] As an advantage of our method results for G_p on all energy scales down to $T = 0$ can be obtained within one approximation scheme and for more realistic lattice models. Furthermore the fRG allows for extensions to non-perfect contacts which have to be considered when comparing with experiments.[5]

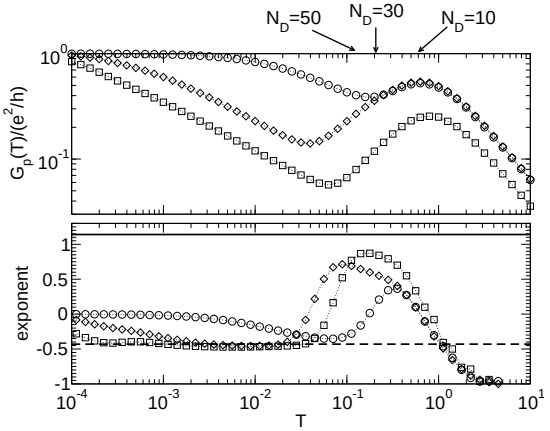

FIG. 3: Upper panel: $G_p(T)$ for $U = 1.5$, $N = 10^4$, $N_D = 10$ with $V_{l/r} = 0.8$ (circles), $N_D = 30$ with $V_{l/r} = 1.5$ (squares), and $N_D = 50$ with $V_{l/r} = 0.8$ (diamonds). The arrows indicate Δ_D. Lower panel: Logarithmic derivative of $G_p(T)$. Solid line: $2\alpha_B^{\rm RG}$; dashed line: $\alpha_B^{\rm RG} - 1$.

We next discuss the case of weak to intermediate barriers, dots of a few ten lattice sites, and larger U. In this part of the parameter space we find non-universal behavior of $G_p(T)$ which so far has not been studied theoretically and provides an alternative interpretation of the QMC data.[10] It might also be relevant in connection with experiments[5] since it is not clear that the experimental dot parameters fall in the regime of universal scaling. In Fig. 3 $G_p(T)$ is shown for $U = 1.5$, $N_D = 10$ with $V_{l/r} = 0.8$ (circles), $N_D = 30$ with $V_{l/r} = 1.5$ (squares), and $N_D = 50$ with $V_{l/r} = 0.8$ (diamonds). These parameter sets are chosen to be close to the set used in the QMC calculations.[10] In the limit of weak barriers and small dots (circles) neither the power-law with the exponent $2\alpha_B$ nor the one with $\alpha_B - 1$ are clearly de-

veloped. For increasing N_D or increasing $V_{l/r}$ the UST regime gets more pronounced. For weak to intermediate barriers no plateau with exponent $2\alpha_B$ is established (see the lower panel). The behavior in the regime of decreasing $G_p(T)$ (for decreasing T) depends on $V_{l/r}$ and N_D and is thus non-universal. It might be identified incorrectly as a power-law with an exponent significantly smaller than $2\alpha_B$, i.e. in the vicinity of $2\alpha_B - 1$.

Our fRG results for $G_p(T)$ in the case of asymmetric barriers and the off resonance scaling of $G(T)$ for both symmetric and asymmetric barriers will be presented in Ref. [17]. For later reference we mention that in all these cases we obtain $T^{2\alpha_B^{\rm RG}}$ for $T \to 0$ as expected.[1]

Using the projection operator onto the subspace of the one-particle states of the dot and the orthogonal complement to the left and right of it the result $|t(\varepsilon,T)|^2 = (4-\varepsilon^2)|\tilde{G}_{1,N}(\varepsilon,T)|^2$ can be written in a form which is useful for obtaining a deeper understanding of the different scaling regimes discussed above and to work out the differences of our approach to the "leading-log" approximation. As an example we take the case of hopping barriers and $N_D = 1$. Then one obtains

$$|t(\varepsilon,T)|^2 = \frac{4\Gamma_l(\varepsilon,T)\Gamma_r(\varepsilon,T)}{\left[\varepsilon - V_g - \Omega_l(\varepsilon,T) - \Omega_r(\varepsilon,T)\right]^2 + \left[\Gamma_l(\varepsilon,T) + \Gamma_r(\varepsilon,T)\right]^2} \quad (3)$$

with $\Gamma_l = t_l^2 \,\mathrm{Im}\,\tilde{G}^0_{j_l-1,j_l-1}$, $\Omega_l = t_l^2 \,\mathrm{Re}\,\tilde{G}^0_{j_l-1,j_l-1}$ and similar expressions for $l \to r$. The Green function $\tilde{G}^0_{i,j}(\varepsilon,T)$ is obtained by considering $\Sigma^{\Lambda=0}$ as an effective potential outside the dot and setting $t_{l/r} = 0$.

For $V_g = 0$, $\varepsilon - V_g - \Omega_l(\varepsilon,T) - \Omega_r(\varepsilon,T)$ vanishes at $\varepsilon = 0$ and we find a resonance. Due to the generalized Breit-Wigner form of Eq. (3) for $t_l = t_r$ the transmission at resonance is 1 independent of the dependence of $\Gamma_{l/r}$ on its arguments and the parameters. It is important to note that in this case and for $T \to 0$, (i) $\Gamma_{l/r}(\varepsilon = 0, T)$ does not follow the single barrier scaling T^{α_B} but instead saturates (even for $N \to \infty$). For asymmetric barriers with $t_r < t_l < 1$ and at resonance $\Gamma_r(\varepsilon,T) \propto T^{\alpha_B^{\rm RG}}$ while (ii) $\Gamma_l(\varepsilon,T)$ increases as $T^{-\alpha_B^{\rm RG}}$. Similar scaling is found for the ε and $1/N$ dependence. These power-laws are cut-off by the largest of the scales T, ε, and Δ_W. Inserting the expressions for $\Gamma_{l/r}$ into Eq. (3) leads to a power-law suppression of $|t(\varepsilon,T)|^2$ with exponent $2\alpha_B^{\rm RG}$ which directly gives $G_p(T) \propto T^{2\alpha_B^{\rm RG}}$ mentioned above. We next study the off resonance case with $V_g \neq 0$ and $t_l = t_r \leq 1$ including the single barrier situation ($t_{l/r} = 1$). Because of the symmetry in the following we suppress the indices l/r. We focus on $T = 0$ and consider $\Delta_W \propto 1/N$ as the relevant energy scale. Then the integral in Eq. (2) can be performed and $|t(0,0)|^2$ is directly related to G. For small V_g we (iii) find $\Gamma(0,0) \propto$ const. and $V_g + 2\Omega(0,0) \propto V_g N^{1-K^{\rm RG}}$, which combines to the expected $1 - G/(e^2/h) \propto N^{2(1-K^{\rm RG})}$. For large V_g, (iv) $\Gamma(0,0) \propto t^2 N^{-\alpha_B^{\rm RG}}$ and $V_g + 2\Omega(0,0) \propto V_g$ which leads to $G \propto N^{-2\alpha_B^{\rm RG}}$. The observations (i)-(iv) are not captured by the parameterization of the effective transmission $|t(\varepsilon,T)|^2$ used in the "leading-log" method.[8, 9, 11] In this approach the important energy dependence of the real part Ω [see (iii) and (iv)] does not appear.

Using Eq. (3) and its generalization for $N_D > 1$[17] the UST regime can be understood quite simply.[18] We here focus on symmetric barriers. Approaching from large T UST sets in at a scale at which only one peak of $|t(\varepsilon,T)|^2$ contributes to the integral in Eq. (2) (respectively for T smaller than the bandwidth at $N_D = 1$). As can be seen in Fig. 2 this scale is significantly smaller than Δ_D. For these $T \gg |\varepsilon|$ we find $\Gamma(\varepsilon,T) \propto t^2 T^{\alpha_B^{\rm RG}}/N_D$. Performing the integral in Eq. (2) leads to $G_p(T) \propto T^{\alpha_B^{\rm RG}-1}$ and $w(T) \propto T$. This scaling continues down to the temperature $T^* \propto (t^2/N_D)^{1/(1-\alpha_B^{\rm RG})}$ at which the width of the peak in $|t(\varepsilon,T)|^2$ is equal to T. This defines the lower bound of the UST regime.

In conclusion, applying the fRG we obtained a comprehensive picture of resonant tunneling in a microscopic model for a Luttinger liquid with $1/2 \leq K \leq 1$. Depending on the dot parameters we found distinctive power-law scaling of $G_p(T)$, but also regimes with non-universal behavior. No signatures of CST were found.

We thank X. Barnabé-Thériault, R. Egger, M. Grifoni, A. Komnik, D. Polyakov, M. Thorwart, and especially H. Schoeller for discussions.

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[18] In contrast to what is found in the model of Ref. [7] for not too small barriers we observe indications of UST with exponent $\alpha_B - 1$ also for $N_D = 1$. At $K = 1/2$, i.e. $\alpha_B = 1$ this leads to a plateau in $G_p(T)$.